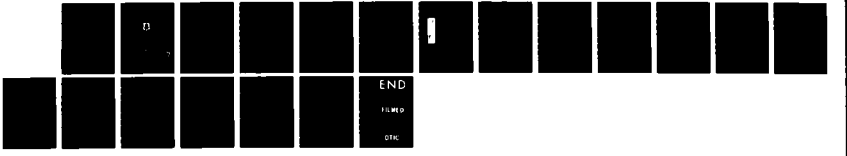
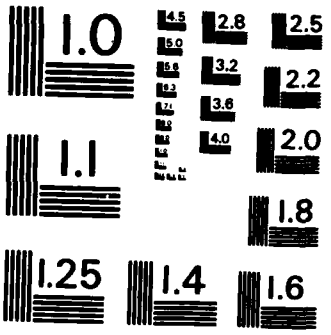
AD-A159 179 NUMERICAL SIMULATION OF DIRECTIONAL SOLIDIFICATION OF CASTINGS(U) FOREIGN TECHNOLOGY DIV WRIGHT-PATTERSON AFB OH Y QUIPING ET AL. 19 AUG 85 FTD-ID(RS)T-0463-85 1/1

UNCLASSIFIED F/G 11/6 NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS - 1963 - A

(2)

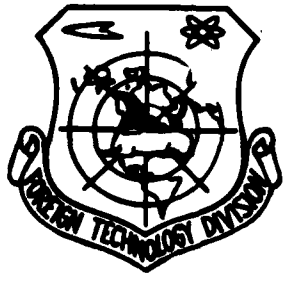
FTD-ID(RS)T-0463-85

FOREIGN TECHNOLOGY DIVISION

NUMERICAL SIMULATION OF DIRECTIONAL SOLIDIFICATION OF CASTINGS

by

Yu Qiuping and Zhou Yaohe



Approved for public release;
distribution unlimited.

EDITED TRANSLATION

FTD-ID(RS)T-0463-85 19 August 1985

MICROFICHE NR: FTD-85-C-000706

NUMERICAL SIMULATION OF DIRECTIONAL SOLIDIFICATION OF CASTINGS

By: Yu Quiping and Zhou Yaohe

English pages: 15

Source: Hangkong Xuebao, Vol. 5, Nr. 3, September 1984, pp. 313-321

Country of origin: China
Translated by: SCITRAN
F33657-84-D-0165
Requester: FTD/TQTA

PREPARED BY:

TRANSLATION DIVISION
FOREIGN TECHNOLOGY DIVISION
WP-AFB, OHIO.

GRAPHICS DISCLAIMER

All figures, graphics, tables, equations, etc. merged into this translation were extracted from the best quality copy available.

FTD 0463-85

Numerical Simulation of Directional Solidification of Castings /313

Northwestern Polytechnical University
Yu Qiuping and Zhou Yaohe

Abstract

Some rules for numerical simulation of the directional solidification process with steep temperature gradient were investigated. In order to improve the accuracy of calculation, the effect of the term ~~$\partial k/\partial T(\partial T/\partial z)^2$~~ in the heat transfer equation on the outcome with steep temperature gradient is discussed. Problems such as how to treat latent heat of solidification, thermal properties at the casting/mold interface and the initial condition are also analyzed. Both finite difference and finite element methods were used to calculate the same casting under identical initial and boundary conditions with the same physical parameters. The results were compared

Table of Symbols

T	temperature (°C)
τ	time (s)
c	specific heat (cal/g°C)
ρ	density (g/cm^3)
k	conductivity coefficient (cal/s.cm°C)
w	heat released by internal source per unit volume and time (cal/s.cm^3)
j	latent heat (cal/g)
f_s	ratio of solidified phase to total amount
c_j	$= -J\ \partial f_s/\partial T$
T_L	liquid phase curve temperature (°C)
T_s	solid phase curve temperature (°C)
b	thermal storage coefficient (cal/cm^2.s$^{1/2}$.°C)
c_p	physical specific heat (cal/g.°C)

received on August 9, 1982

M	$= \Delta\tau.k/c.\rho.(\Delta x)^2$, $\Delta\tau$ is the time interval and Δx is the step length in space
p	superscript of T representing time interval
i	step number in z-direction
j	step number in r-direction
m	slope of liquid phase curve

C_0	percentage of solute concentration /314
k_0	distribution index

Subscripts

m or M	castings
s	mold
if	interface

I. Introduction

Computer numerical simulation of the solidification process is a new subject of study in casting. In recent years, its scope and width have been expanding rapidly. One of the directions is to study the directional solidification process of castings by numerical simulation.

One of the key problems in conducting numerical simulation for the solification process is the selection of thermodynamic parameters for the castings and molds. After taking into account that there is very little data on directionally solidified high temperature alloys and molds, A1-4.5Cu alloy was chosen in this work. The mold is also metallic, which is a new trend in directional solidification.

In the solidification process, the bottom of the mold was cooled while it was heated all the way around. The simulation condition is casting temperature 740°C, mold preheating temperature (measured 4cm from the bottom) 650°C and water cooled crystallized (200 1/hr). The axial temperature gradient was found to be 30-60°C/cm experimentally. The specimen is a 3cm

diameter 10cm long cylinder. The columnar structure is shown in Figure 1[1].

Figure 1. Columnar Structure of the Test Ingot

II. Basic Equations /315

Due to the fact that the melting point of the aluminum alloy used in the experiment is not very high (not exceeding 750°C), the temperature differential in directional solidification is relatively small. After neglecting radiation and converting convection to conduction, the complicated heat transfer problem is simplified to a simple conduction problem.

The basic heat transfer equation is as follows:

$$c\rho\frac{\partial T}{\partial \tau} = \nabla\cdot(k\nabla T) \qquad (1)$$

For an axial symmetric object, equation (1) can be expressed in cylindrical coordinates

$$c\rho\frac{\partial T}{\partial \tau}=\frac{1}{r}\ \frac{\partial}{\partial r}\left(rk\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(k\ \frac{\partial T}{\partial z}\right) \qquad (2)$$

Both finite difference and finite element methods were used to calculate the same casting under the same condition. The meshes for the casting and the mold are shown in Figures 2 and 3. The discrete elements are not the same for those two methods.

From equation(2),the numerical equation for the finite difference method is

$$T^{n+1}_{i,j}=4MT^{n}_{i,j+1}+MT^{n}_{i+1,j}+MT^{n}_{i-1,j}+(1-6M)T^{n}_{i,j}+\theta_k\left(\frac{T^{n}_{i-1,j}-T^{n}_{i+1,j}}{2\Delta r}\right)^2 \qquad (3)$$

$j>1$

$$T^{n+1}_{i,j}=\left[1-\frac{1}{2(j-1)}\right]MT^{n}_{i,j-1}+\left[1+\frac{1}{2(j-1)}\right]MT^{n}_{i,j+1}+MT^{n}_{i-1,j}$$
$$+MT^{n}_{i+1,j}+(1-4M)T^{n}_{i,j}+\theta_k\left(\frac{T^{n}_{i-1,j}-T^{n}_{i+1,j}}{2\Delta r}\right)^2$$

$$\theta_k=\frac{\Delta\tau}{c\rho}\ \frac{\partial k}{\partial T}. \qquad (4)$$

where $\theta_k = \Delta\tau/c\rho\ \ \partial k/\partial T$.

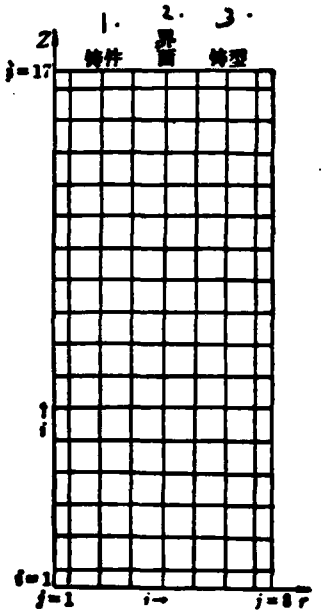


Figure 2. Mesh for Finite Difference Method

Key: 1. casting
2. interface
3. mold

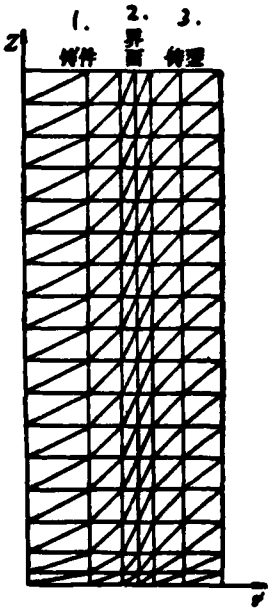


Figure 3. Mesh for Finite Element Method

Key: 1. casting 2. interface 3. mold

The term $\theta_k(T^p_{i-1,j}-T^p_{i+1,j}/2\Delta r)$ in equations (3) and (4) is a result of taking $\partial k/\partial T(\partial T/\partial Z)^2$ into consideration. Because the rate of change of k with respect to T is usually small, and the temperature gradient in sand mold casting is not very high, the square term of this temperature gradient can be omitted in numerical calculation using finite difference. This has very little effect on the accuracy of calculation for sand mold casting. /316

However, it is not appropriate to neglect the temperature gradient square term in the basic equation in a relatively slow solidification process with large temperature gradient. The axial temperature gradient is always very large in casting ingots. Whether to include the term $\partial k/\partial T(\partial T/\partial Z)^2$ has a significant effect on the accuracy of the calculation. According to the results shown in Figure 4, the calculated result deviates positively from the experimental value when $\theta_k = 0$, i.e., neglecting the square of the temperature gradient term. If $\theta_k = -0.00002$ chosen properly, a negative deviation would result, such as in the case $\theta_k = -0.000094$. It was estimated that $\theta_k = -0.00002$ from the k vs T curve for this aluminum alloy. Strictly speaking, θ_k should also be a function of T because k is a function of T.

The numerical equation for equation (2) in the finite element method:

$$\left[H+\frac{2}{\Delta\tau}P\right]\{T\}_\tau+\left[H-\frac{2}{\Delta\tau}P\right]\{T\}_{\tau-\Delta\tau}+\{Q\}_{\tau-\Delta\tau}+\{Q\}_\tau=0 \quad (5)$$

where H is a matrix related to the thermal conductivity coefficient, P is a matrix related to specific heat and density and Q is series related to the natural boundary condition. Hence, $\{T\}_\tau$ can be obtained by solving the set of linear equations when $\{T\}_{\tau-\Delta\tau}$ is known.

In the finite element method, it was assumed that there was no heat flux across axisymmetric lines, i.e., an adiabatic process. The treatment involves the use of a third type of boundary condition: $-k\,\partial T/\partial r\big|_{axial} = 0$[3]. In our work, the first type

of boundary condition is used on three other sides. Along the axis, v = 0. Thus, equation (5) can be simplified:

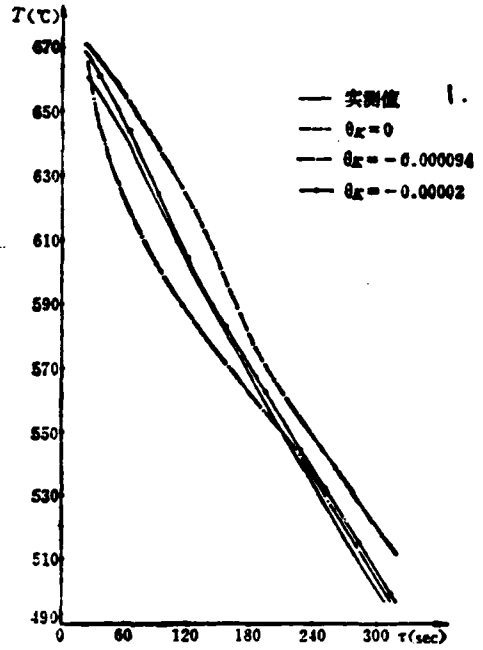


Figure 4. Comparison Between Simulated Temperatures with Different Values of θ_k and its Experimental Data (at Z = 5.1cm)

Key: 1. experimental value

$$\left[H+\frac{2}{\Delta\tau}P\right]\{T\}_{\cdot}+\left[H-\frac{2}{\Delta\tau}P\right]\{T\}_{\cdot\cdot\cdot}=0 \qquad (6) \quad /317$$

This is the equation used in this work.

Because physical parameters of the material such as k, c, and p are functions of T, therefore, the matrices [H] and [P] vary with T[4].

The following is a comparison of these two methods.

The explicit finite difference method is more accurate when its stability condition is met. Furthermore, there is no matrix in the process. The storage requirement is small. However, the time interval is limited by the stability requirement.

Because an element can be divided arbitrarily in the finite element method, it is more superior in dealing with a castings of complex shape. A simple triangular element method was used with linear intrapolation, therefore, the error is larger.

Figure 5 is a comparison of these two methods against the experimental result.

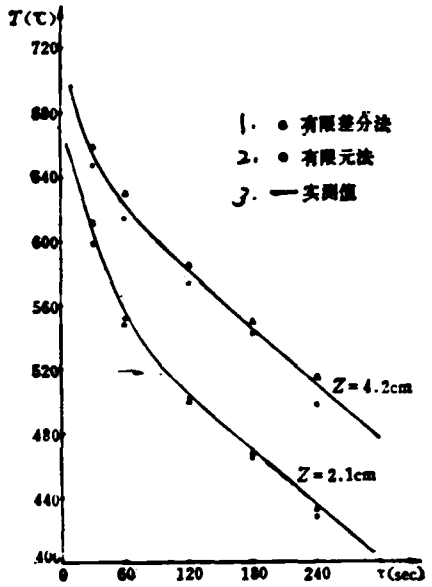


Figure 5. Comparison Between the Results of the Two Computation Methods and Experimental Data

Key:
1. finite difference method
2. finite element method
3. experimental value

III. Treatment of Several Specific Problems

1. Latent Heat

Latent heat must be considered in the heat transfer process of cast solidification. The latent heat of crystallization is high for metals and alloys. For example, it is 92.0 cal/g for Al-4.5Cu. If the liquid-solid line spacing is 103°C and the specific heat is 0.31 cal/g°C, then the heat of solidification 31.9cal./g,

stage will affect the accuracy of calculation.

If there is a heat source in the object, then the expression for equation (1) becomes

$$c\rho\frac{\partial T}{\partial \tau} = \nabla\cdot(k\nabla T) + w \tag{7}$$

Let us assume that the latent heat is a heat source in the solidification stage and the amount of heat released is proportional to the percentage of solid precipitated per unit time, i.e.,

$$w = \rho J\frac{\partial f_s}{\partial \tau} \tag{8}$$

Usually, f_s is also a function of T and T is a function of coordinate and time. Therefore:

$$\frac{\partial f_s}{\partial \tau} = \frac{\partial f_s}{\partial T}\ \frac{\partial T}{\partial \tau}$$

$$w = \rho J\frac{\partial f_s}{\partial T}\ \frac{\partial T}{\partial \tau}$$

Substituting the above into equation (7), we get

$$\left(c - J\frac{\partial f_s}{\partial T}\right)\rho\ \frac{\partial T}{\partial \tau} = \nabla(k\nabla T) \tag{9}$$

/318

Let

$$c_j = -J\frac{\partial f_s}{\partial T} \tag{10}$$

then, the specific heat c in the solidification process should include the physical specific heat c_p and the latent heat specific heat c_j, i.e.,

$$c = c_p + c_j \tag{11}$$

This is the so-called reduced specific heat method which is applicable to alloys of a certain crystallization temperature range.

The simplest treatment is

$$f_s = \frac{T_L - T}{T_L - T_s} \tag{12}$$

The result is $c_j = J/T_L - T_S$ which is a mean formula.

If we combine this with the binary diagram of an alloy, another type of formula can be obtained. For instance,

$$f_s = \frac{T_L - T}{(1-k_0)(mC_0 + T_L - T)} \quad (13)$$

where the lever law in equilibrium was used in the derivation of equation (13).

The distribution of the solidified solid phase is related to the heat exchange of the system. When the temperature drops slowly near equilibrium, existing diagrams can be used to obtain an expression for f_s. The situation is more complicated for non-equilibrium conditions.

The non-equilibrium solidification problem in directional crystallization can be treated according to the normal solidification equation

or

$$C_L = C_0 f_L^{k_0 - 1}$$

$$f_L = \left(\frac{T_m - T}{T_m - T_L}\right)^{\frac{1}{k_0 - 1}} \quad (14)$$

where T_m is the melting point of the base metal in the alloy. The relation between f_S and temperature T can be obtained based on $f_s = 1 - f_L$.

Three types of reduced specific heat formulas were used to simulate the same casting condition.

(1) reciprocal square formula obtained from eq. (14)

$$c_j = \frac{mC_0 J}{(1-k_0)(mC_0 + T_L - T)^2}$$

(2) equation of average derived from eq. (13)

$$c_j = \frac{J}{T_L - T_s}$$

(3) trapezoidal equation, i.e., the slope of c_j vs T line is different in various temperature intervals.

Equation (10) shows that the simulation of latent heat is only accurate when the f_s vs T relation is known for the entire solidification process. A feasible method is to find the f_s vs T curve experimentally. The trapezoidal equation is obtained from the f_s-T curve of the Al-4.5Cu alloy.

Normally, although the temperature field may differ by using a different formula to simulate the latent heat of the case, however, it has little effect on the outcome. In directional solidification, external conditions are controlled rigorously. One can see from the simulation results that different latent heat formulas would yield different isothermal solid-liquid interface curvature and solidification zone width. Therefore, the solidification of latent heat must be handled well in directional solidification. Otherwise, wrong results may be obtained.

Figure 6 shows the isothermal surfaces between liquidus and solidus of ingot 40 and 60 seconds after casting with different latent heat formulas. The * symbol respresents an actual experimental point of liquidus in the casting and the symbol • represents an experimental solidus point. One can see that it is more appropriate to use the trapezoidal formula.

2. Heat Transfer at the Interface /319

For convenience, it is usually classified as ideal and non-ideal contacts. In reality, ideal contact is rare. In order to improve the accuracy of calculation, the study of non-ideal contact is receiving more attention. At high temperature, the physico-chemical process at the interface is very complex. The mechanism causing heat transfer variation is not very clear. Mold coating, oxide layer on the case and gap created in solidification will change the heat transfer at the interface.

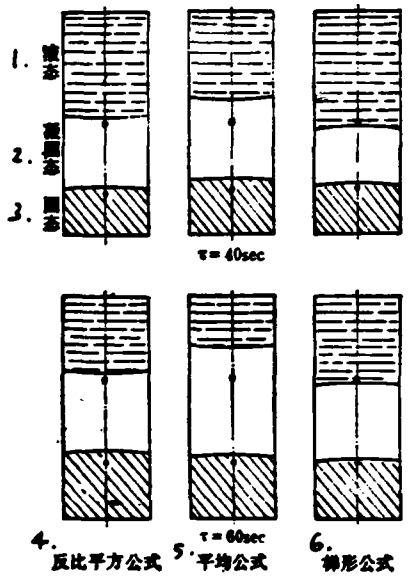


Figure 6. Influence of Different Formulae for Latent Heat on the Isothermal Surface Between Liquidus and Solidus

Key:

1. liquidus
2. solidified phase
3. solidus
4. reciprocal square formula
5. average formula
6. trapezoidal formula

Interfacial heat transfer may be simulated using different formulas. In the finite difference method, a reduced thermal conductivity coefficient method is usually used. Its formula is as follows:

$$k_{ij} = K\frac{2k_m k_s}{k_m + k_s} \tag{15}$$

where k is a correction factor. In ideal contact situations, k = 1.

In the finite element method, the non-ideal contact is corrected by modifying the thermal conductivity coefficient of the mold element at the interface[7].

3. Initial Condition

The difficulty in determining the initial condition is to calculate the temperature at the mold and casting interface. In sand casting, the following formula is used to obtain the initial interfacial temperature.

$$T_{ij}=\frac{b_M T_{MI}+b_S T_{SI}}{b_M+b_S} \tag{16}$$

where T_{MI} and T_{SI} are the initial temperature of the casting and mold, respectively.

There is some deviation when equation (16) is used in a directional solidification process with steep temperature gradient. The reason is that the formula does not include the latent heat released by some solidified metal near the initial interface. Equation (16) is corrected by this effect:

$$T_{ij}=\frac{b'_M T_{MI}+b_S T_{SI}}{b'_M+b_S} \tag{17}$$

where $b'_M = [k_M P_M (c_M + J/T_L - T_S)]^{1/2}$. Other formulas taking released latent heat include

$$T_{ij}=\frac{\rho_M c_M T_{MI}+\rho_S c_S T_{SI}+T_L \rho_M J/(T_L-T_S)}{\rho_M c_M+\rho_S c_S+\rho_M J/(T_L-T_S)} \tag{18}$$

The following table lists the initial temperature values calculated with three above formulas, as well as the experimental value (condition: casting temperature of the ingot and pre-heating temperature of the crystallizer are known). Equation (17) gives the most close result as compared to the measured value.

Temperature °C formula	condition	casting temperature 740°C crystallizer temperature 520°C
Calculated based on eq (16)		598
Calculated based on eq (17)		635
Calculated based on eq (18)		642
Experimental		630

Conclusions

/320

1. In order to improve the accuracy of numerical simulation of the solidification process with steep temperature gradient, the temperature graient square terms such as $\partial k/\partial T(\partial T/\partial Z)^2$ in the heat transfer equation cannot be neglected.
2. Different formulas to deal with latent heat will have different effects on the isothermal surface and zone width.
3. The calculation of the initial temperature at the casting mold interface must take the latent heat released by the casting into consideration when the temperature gradient is steep.
4. There are advantages and disadvantages in both methods. Finite difference is more accurate when the stability requirement is met. It is suited for small computers because the storage requirement is small. Finite element is suited for castings of complicated shape because elements can be divided arbitrarily.

References

[1] He Qingfeng, Effect of Solidification Condition on Structure and Properties of Al-4.5Cu Alloy, Master's Thesis of Northwestern Polytechnical University, (1981).

[2] Zhu Bofang, Principle and Application of Finite Element Method, Hydroelectric Power Publishing Co., (1979), pp 251-260.

[3] Mathew, J. and Brody, H.D., Analysis of Heat Transfer in Continuous Casting Using a Finite Element Method,

Conference on Computer Simulation for Materials Applications, (1976), p. 1142.

[4] Comini, G., Delguidice, S., Lewis, R.W. and Zienkiewicz, O.Z., Finite Element Solution of Non-Linear Heat Conduction Problems with Special References to Phase Change, Inter. Journal of Numerical Methods in Eng., Vol. 8, (1974), pp. 613-624.

[5] Guo Keren, Jin Junzhe, et al, Mathematical Modeling of Solidification of Large Scale Casting, Dalian Engineering Institute Journal, 2(1980), pp 1-17.

[6] Clyne, T.W. and Davies, G.J., The Influence of Composition on Solidification Cracking Susceptibility in Binary Alloy Systems, The British Foundreyman, Vol. 74, Apr. (1981), p. 65.

[7] Pehlke, R.D., Kirt, M.J., Marrone, R.E., and Cook, D.J., Numerical Simulation of Casting Solidification, AFS Cast Metals Research Journal, Vol. 9, June (1973), pp 49-55.

END

FILMED

10-85

DTIC